

10/513699

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information
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NEWS 9 APR 28 Limits doubled for structure searching in CAS
REGISTRY
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STN Easy
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introduction of free HIT display format
NEWS 14 MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal
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NEWS 15 MAY 28 CAS databases on STN enhanced with NANO super role in
records back to 1992
NEWS 16 JUN 01 CAS REGISTRY Source of Registration (SR) searching
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NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
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FILE 'HOME' ENTERED AT 15:50:28 ON 22 JUN 2009

=> file reg		
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FILE 'REGISTRY' ENTERED AT 15:52:03 ON 22 JUN 2009
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STRUCTURE FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5
DICTIONARY FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

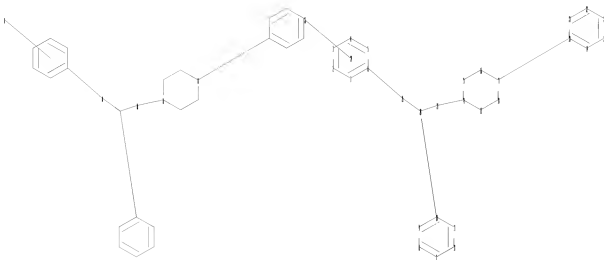
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<http://www.cas.org/support/stngen/stdoc/properties.html>

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Uploading C:\Program Files\Stnexp\Queries\10594105species.str

10/513699



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chain nodes :
25 26 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-28 14-27 17-20 25-28 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-27 15-16 16-17 17-18 17-20 25-28 27-28
exact bonds :
10-28
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :
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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:Atom
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10/513699

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

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FULL SCREEN SEARCH COMPLETED - 11045 TO ITERATE

100.0% PROCESSED 11045 ITERATIONS

88 ANSWERS

SEARCH TIME: 00.00.01

L2 88 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.84

187.50

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FILE COVERS 1907 - 22 Jun 2009 VOL 150 ISS 26

FILE LAST UPDATED: 21 Jun 2009 (20090621/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l2 full
L3 2 L2

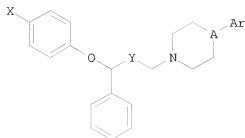
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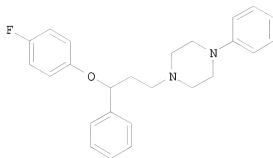
Erich Leese

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:1103625 CAPLUS
 DOCUMENT NUMBER: 143:387060
 TITLE: Preparation of piperazine or piperidine derivatives as
 serotonin reuptake inhibitors
 INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey,
 James Michael
 PATENT ASSIGNEE(S): Baylor University, USA
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA			
EP 1732610	A2	20061220	EP 2005-730778	20050328
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P	P 20040326
			WO 2005-US10356	W 20050328
OTHER SOURCE(S):	CASREACT 143:387060; MARPAT 143:387060			
GI				



I



II

AB Title compds. I [X = F or CF₃; Y = (CH₂)_n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC₅₀ values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

IT 691872-56-7P 691872-58-9P 691872-60-3P
691872-62-5P 691872-64-7P 691872-66-9P
866548-21-2P 866548-22-3P 866548-24-5P
866548-25-6P

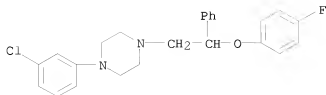
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

RN 691872-56-7 CAPLUS

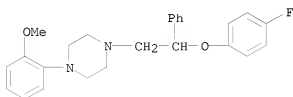
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)

10/513699



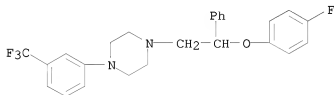
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-
(CA INDEX NAME)



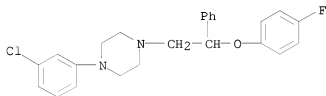
RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 691872-62-5 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

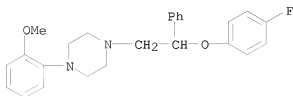
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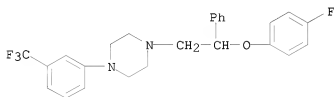
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS

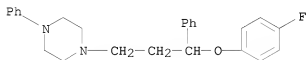
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 866548-21-2 CAPLUS

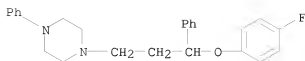
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl- (CA INDEX NAME)



RN 866548-22-3 CAPLUS

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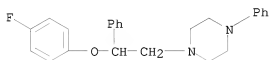
10/513699



● HCl

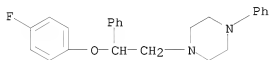
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CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl- (CA INDEX NAME)



RN 866548-25-6 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:170822 CAPLUS

DOCUMENT NUMBER: 140:417233

TITLE: Synthesis and biological evaluation of 2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile
 AUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas V.; Pinney, Kevin G.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and The Center for Drug Discovery, Baylor University, Waco, TX, 76798-7348, USA

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6), 1483-1491

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:417233

AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-piperazine, modeled after the potent antidepressant fluoxetine and coupled with several functionalized piperazines, have been prepared by chemical synthesis as selective serotonin reuptake inhibitors (SSRIs) with a potentially improved adverse reaction profile. Typical SSRIs, although very effective in the treatment of depression, still face the troublesome side effect of sexual dysfunction. A number of pharmacol. agents-notably, drugs in the piperazine class-have been used to reverse SSRI-induced sexual dysfunction, and evidence for developing an improved SSRI by coupling a fluoxetine congener with the pharmacophore of a reversal agent holds promise. Preliminary data indicates that the hydrochloride (HCl) salts of piperazines exhibit single-site binding at the site of the serotonin reuptake transporter (SERT). However, each of the three compds. are much less potent than typical SSRIs, showing micromolar (μM) affinity for the SERT with IC_{50} values of 1.45 μM , 3.27 μM , and 9.56 μM , resp. Further biol. evaluation of piperazine compds. is needed before definitive conclusions can be made with regard to each compound's potential for use as an SSRI-type candidate which is devoid of sexual side effects. Nevertheless, the initial findings are quite encouraging, thus lending credence to the idea of hybridizing an SSRI congener with that of the pharmacophore of an agent known to reverse or treat SSRI-induced sexual dysfunction.

IT 691872-62-5P 691872-64-7P 691872-66-9P

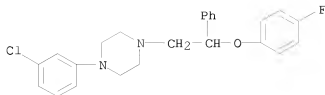
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-62-5 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)

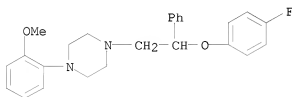
10/513699



● HCl

RN 691872-64-7 CAPLUS

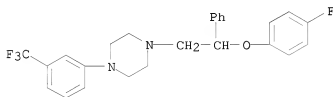
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

IT 691872-56-7P 691872-58-9P 691872-60-3P

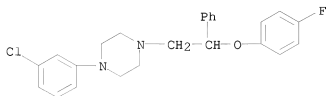
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-56-7 CAPLUS

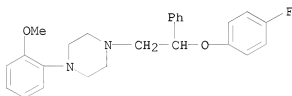
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CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



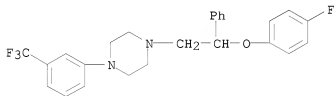
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d his

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FILE 'REGISTRY' ENTERED AT 15:52:03 ON 22 JUN 2009

L1 STRUCTURE UPLOADED

L2 88 S L1 FULL

FILE 'CAPLUS' ENTERED AT 15:53:50 ON 22 JUN 2009

L3 2 S L2 FULL

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

20.28

207.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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-1.64

-1.64

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